Decay of Superconducting and Magnetic Correlations in One- and Two-Dimensional Hubbard Models[1]

Tohru Koma[2] and Hal Tasaki[3]

Department of Physics, Gakushuin University, Mejiro, Toshima-ku, Tokyo 171, JAPAN

Abstract

In a general class of one and two dimensional Hubbard models, we prove upper bounds for the two-point correlation functions at finite temperatures for electrons, for electron pairs, and for spins. The upper bounds decay exponentially in one dimension, and with power laws in two dimensions. The bounds rule out the possibility of the corresponding condensation of superconducting electron pairs, and of the corresponding magnetic ordering. Our method is general enough to cover other models such as the t-J model.

The Hubbard model and its variants have been attracting considerable interest. But rigorous results are still rare. In one dimension, the Bethe ansatz method has been successfully applied [1] both to the ground state and to the finite temperature Gibbs state. In general dimensions, Lieb's theorem [2] and Nagaoka's theorem [3] on the ground state structures are known. In one and two dimensions, Ghosh [4] proved the absence of magnetic ordering at finite temperatures.

In the present letter, we extend McBryan and Spencer's method [5] developed in classical spin systems to a general class of Hubbard models in one and two dimensions, and prove upper bounds for various correlation functions at finite temperatures. The bounds rule out the possibility of magnetic ordering and condensation of electrons or superconducting electron pairs such as Cooper pairs or η-pairs [6].

We consider a tight binding electron model on the one dimensional lattice $\mathbf{Z}$ or the square lattice $\mathbf{Z}^2$ [7]. The Hamiltonian is given by

$$H = -\sum_{x,y\in\mathbf{Z}^d}\sum_{\sigma=\uparrow,\downarrow} t_{x,y}c^\dagger_{x,\sigma}c_{y,\sigma} + V(\{n_{x,\sigma}\}) + \sum_{x\in\mathbf{Z}^d}\mathbf{h}_x\cdot\mathbf{S}_x, \tag{1}$$

with $d = 1$ or 2. The number operators are defined by $n_{x,\sigma} = c^\dagger_{x,\sigma}c_{x,\sigma}$, and spin operators by $S^j_x = \sum_{\sigma,\sigma'=\uparrow,\downarrow} c^\dagger_{x,\sigma}\tau^j_{\sigma,\sigma'}c_{x,\sigma'}$ $(j = 1, 2, 3)$, where $(\tau^j_{\sigma,\sigma'})_{\sigma,\sigma'=\uparrow,\downarrow}$ are Pauli spin matrices and $c^\dagger_{x,\sigma}$, $c_{x,\sigma}$, are the creation and the anihilation operators, respectively, for the electron at site

[1] Published in Phys. Rev. Lett. **68**, 2348 (1992). Reference [17] (which appeared after the publication) was added in the archived version.

[2] koma@riron.gakushuin.ac.jp

[3] hal.tasaki@gakushuin.ac.jp, http://www.gakushuin.ac.jp/˜881791/halE.htm

x with spin σ. The hermitian hopping matrix (t_{xy}) is arbitrary, except for the conditions that there are finite constants t, R, and $|t_{xy}| \leq t$ holds for any x, y, and t_{xy} is vanishing [8] for $|x-y| \geq R$. Note that we can include external magnetic field which is represented by complex t_{xy}. The interaction $V(\{n_{x,\sigma}\})$ is an arbitrary function of the number operators, and $\mathbf{h}_x$ represents local magnetic field or spin-flip impurity. Note that the Hamiltonian (1) is not necessarily completely isotropic in spin space, but has a global $O(2)$ symmetry related to the spin rotation about the z-axis. We stress that the class of Hamiltonians considered here includes not only the well studied models like the (standard) Hubbard model or the periodic Anderson model, but also many of their variants with , e.g., long-range, random or spin-dependent interactions.

To define the Gibbs state, we replace the infinite lattice with a finite lattice of linear dimension L with periodic boundary conditions. The thermal expectation value of an arbitrary operator A is defined by

$$\langle A \rangle_L = \frac{\mathrm{Tr}(Ae^{-\beta H})}{\mathrm{Tr}(e^{-\beta H})}, \tag{2}$$

where the trace is over all the electron states. We consider the infinite volume state defined by

$$\langle A \rangle = \lim_{L\to\infty} \langle A \rangle_L \,, \tag{3}$$

with the electron density fixed to ρ. Our result is independent of ρ and thus applies to grand canonical averages as well.

The main result of the present letter is the following.

Theorem: There exist finite constants [9] α, γ, δ and a function $f(\beta)$ which depend only on the hopping matrix (t_{xy}). The function $f(\beta)$ is decreasing and behaves as $f(\beta) \approx 1/\beta$ for $\beta \gg \delta$ and $f(\beta) \approx (2/\delta)|\ln \beta|$ for $\beta \ll \delta$. In a two dimensional model in the class described above, we have

$$\left|\left\langle c^\dagger_{x,\uparrow} c^\dagger_{x,\downarrow} c_{y,\uparrow} c_{y,\downarrow} + \mathrm{H.c.}\right\rangle\right| \;\leq\; 2|x-y|^{-\alpha f(\beta)}, \tag{4}$$

$$\left|\left\langle c^\dagger_{x,\sigma} c_{y,\sigma} + \mathrm{H.c.}\right\rangle\right| \;\leq\; 2|x-y|^{-\alpha f(2\beta)/2}, \tag{5}$$

for any finite β and for any x, y with sufficiently large $|x-y|$. If the local field has the form $\mathbf{h}_x = (0, 0, h_x)$ we further have

$$\left|\left\langle S^1_x S^1_y + S^2_x S^2_y \right\rangle\right| \leq |x-y|^{-\alpha f(\beta)}, \tag{6}$$

for any finite β and for any x, y with sufficiently large $|x-y|$. In a one dimensional model, we have the above bounds (4), (5) and (6) with the right-hand-sides replaced with $2\exp[-\gamma f(\beta)|x-y|]$, $2\exp[-\gamma f(2\beta)|x-y|/2]$ and $\exp[-\gamma f(\beta)|x-y|]$, respectively.

The above bounds rigorously rule out the possibility of the corresponding condensations of electrons or electron pairs and of the corresponding magnetic ordering. The bound (4), for example, inhibits the condensation of singlet electron pairs such as the Cooper pairs or the η-pairs [6]. However our method can be easily extended to rule out any kind of condensation which is related to a spontaneous breakdown of the quantum mechanical global $U(1)$ symmetry. It is also straightforward to extend the method to cover other systems such as the Hubbard model with nonlocal spin-flip term or the t-J model [10]. The explicit upper bounds for the correlation functions provide further information about the propagation of electrons, electron pairs and magnons. The astonishing generality of the theorem, especially the complete arbitrariness of interactions, may be regarded as a sharp demonstration of the fact that the electron hopping plays a fundamental role in various condensation phenomena in itinerant electron systems.

The power law decaying upper bounds in the theorem are certainly not optimal at high temperatures, where one generally expects to have exponential decay. Even in low temperatures, a class of models which are sufficiently close to the antiferromagnetic Heisenberg model is expected to show exponential decay. Among the varieties of models covered by the theorem, however, one might well find those which exhibit "exotic" phase transitions leading to power law decay. It is notable that the power indices in the upper bounds (4), (5), (6) are proportional to β^{-1} at low temperatures. This means that the slowest possible decay in these models is of the Kosterlitz-Thouless type. In one dimension, the exponentially decaying upper bounds in the theorem provide upper bounds for various correlation lengths. The bounds, which are proportional to β^{-1} at low temperatures and to $|\ln \beta|$ at high temperatures, reproduce a typical crossover behavior of correlation lengths in one dimensional tight-binding electron systems.

Our proof is based on the method developed by McBryan and Spencer [5] for classical spin systems, and on its extension to quantum spin systems by Ito [11]. In these works, the global continuous symmetry of the spin space played an essential role [12]. Our strategy here is to make use of the global $U(1)$ symmetry related to the quantum mechanical phase. In this approach, we do not have to make further assumptions on the symmetry of the system since the $U(1)$ symmetry exists in any quantum particle systems. We believe that the present method can be extended to much larger class of quantum particle systems. In the present letter, we restrict ourselves to the lattice fermion problems, which are free from ultraviolet divergence.

The absence of magnetic ordering in one and two dimensions was proved by Ghosh [4], who extended the Bogoliubov inequality method of Mermin and Wagner's [13]. We note that, by combining the Mermin-Wagner argument with the idea to make use of the quantum mechanical $U(1)$ symmetry, one can also prove the absence of condensation of electron pairs (or electrons). To do this, one should replace the operators A and B in [4] with the Fourier transforms of the number operator $n_x = n_{x,\uparrow} + n_{x,\downarrow}$ and of the order variable $O_x = c_{x,\uparrow} c_{x,\downarrow}$

(or $c_{x,\sigma}$), respectively. We also note that the Mermin-Wagner argument can be extended to cover non-translation-invariant models as those considered here.

In what follows, we describe the proof of the bound (4) in detail. We first prove the bound in a finite periodic lattice of linear dimension L, and then take the limit $L \to \infty$. To make use of the global quantum mechanical symmetry, we note that the $U(1)$ gauge transformation is represented by the unitary operator

$$G(\theta) = \prod_{u,\sigma} \exp[-i\theta_u n_{u,\sigma}], \tag{7}$$

where $\theta = \{\theta_u\}$ is an arbitrary real function on the lattice. In the following, however, we let θ_u to be pure imaginary, in which case the operator $G(\theta)$ is no longer unitary. Since $G(\theta)$ is invertible, we have

$$\mathrm{Tr}[Ae^{-\beta H}] = \mathrm{Tr}\left[G(\theta)AG(\theta)^{-1}\exp[-\beta G(\theta)HG(\theta)^{-1}]\right], \tag{8}$$

for arbitrary complex θ_u. Here the transformed Hamiltonian is

$$G(\theta)HG(\theta)^{-1} = -\sum_{u,v,\sigma} t_{u,v}\, e^{-i(\theta_u-\theta_v)} c^\dagger_{u,\sigma}c_{v,\sigma} + V(\{n_{u,\sigma}\}) + \sum_u \mathbf{h}_u \cdot \mathbf{S}_u. \tag{9}$$

Let $\varphi = \{\varphi_u\}$ be a real function which will be specified later. We consider the operator $G(-i\varphi)$ obtained by setting $\theta = -i\varphi = \{-i\varphi_u\}$ in (7). Let us fix lattice sites x, y, and take $A = c^\dagger_{x,\uparrow}c^\dagger_{x,\downarrow}c_{y,\uparrow}c_{y,\downarrow}$. Straightforward calculations show

$$G(-i\varphi)AG(-i\varphi)^{-1} = \exp[-2(\varphi_x - \varphi_y)]A, \tag{10}$$

and

$$G(-i\varphi)HG(-i\varphi)^{-1} = H + U + iP, \tag{11}$$

where

$$U = -\sum_{u,v,\sigma} t_{u,v}\{\cosh(\varphi_u - \varphi_v) - 1\}c^\dagger_{u,\sigma}c_{v,\sigma}, \tag{12}$$

and

$$P = -i\sum_{u,v,\sigma} t_{u,v}\sinh(\varphi_u - \varphi_v)c^\dagger_{u,\sigma}c_{v,\sigma} \tag{13}$$

are hermitian matrices.

We can bound the right-hand-side of (8) as

$$\begin{aligned}
&\left|\mathrm{Tr}\left[G(-i\varphi)AG(-i\varphi)^{-1}\exp[-\beta G(-i\varphi)HG(-i\varphi)^{-1}]\right]\right| \\
&\le e^{-2(\varphi_x-\varphi_y)}(\|A^*A\|_\infty)^{1/2}\mathrm{Tr}[e^{-(\beta GHG^{-1})/2}e^{-(\beta G^{-1}HG)/2}] \\
&\le e^{-2(\varphi_x-\varphi_y)}\mathrm{Tr}[e^{-\beta(H+U)}] \\
&\le e^{-2(\varphi_x-\varphi_y)}\|e^{\beta U}\|_\infty \mathrm{Tr}[e^{\beta H}],
\end{aligned} \tag{14}$$

where $\|O\|_\infty$ denotes the maximum of the absolute values of the eigenvalues of a hermitian matrix O. To prove the above bounds, we use the following inequalities for operators (matrices) on a finite dimensional space. i) The Schwartz inequality; $\mathrm{Tr}[OP] \le \{\mathrm{Tr}[O^*O]\mathrm{Tr}[P^*P]\}^{1/2}$ with O, P arbitrary. ii) $|\mathrm{Tr}[OP]| \le \|O\|_\infty \mathrm{Tr}[P]$ with O hermitian and P positive. iii) $\mathrm{Tr}[(O^*)^N O^N] \le \mathrm{Tr}[(O^*O)^N]$ with$N = 2^m$ and O arbitrary [14]. iv) The Golden-Symanzik-Thompson inequality [15] $\mathrm{Tr}[e^{O+P}] \le \mathrm{Tr}[e^O e^P]$ where O, P hermitian. To show the first bound in (14), we set $W = \exp[-\beta G(-i\varphi) H G(-i\varphi)^{-1}/2]$, $A' = G(-i\varphi) A G(-i\varphi)^{-1}$, and use i) and ii) to get

$$\begin{aligned}\mathrm{Tr}[(A'W)W] &\le (\mathrm{Tr}[A'^* A' W W^*]\mathrm{Tr}[WW^*])^{1/2} \\ &\le (\|A'^* A'\|_\infty)^{1/2} \mathrm{Tr}[WW^*].\end{aligned} \tag{15}$$

The second bound follows by noting that $\|A\|_\infty = 1$, and setting

$$X = \exp\left[-\frac{\beta G(-i\varphi) H G(-i\varphi)^{-1}}{2N}\right], \tag{16}$$

to get $\mathrm{Tr}[X^N (X^*)^N] \le \mathrm{Tr}[(XX^*)^N]$ from iii). The right hand side converges to $\mathrm{Tr}[\exp[-\beta(H+U)]]$ as $N \to \infty$. The third bound is an easy consequence of iv) and ii).

Now we choose φ. Let λ_{uv} be real hopping matrix elements that satisfy $\lambda_{uv} = \lambda_{vu} \ge |t_{uv}|$, and $\lambda_{uv} = 0$ for $|u - v| \ge R$. We further require λ_{uv} to be periodic, i.e., there are positive integers p, q, and $\lambda_{uv} = \lambda_{u+d,v+d}$ holds for any $d = mpe_1 + mqe_2$ where m, n are arbitrary integers and e_1, e_2 are two unit vectors of the lattice. (In one dimension, we of course set $d = mpe_1$.) We assume that the lattice size L is a common multiple of the periods p, q. The conditions imposed on t_{uv} ensures the existence of such λ_{uv}. (The simplest choice, which is always possible, is $\lambda_{uv} = t$ for $|u - v| < R$, and $\lambda_{uv} = 0$ otherwise. By choosing λ_{uv} which is "closer" to t_{uv}, however, one gets better constants in the resulting bounds.) Let $f = \{f_u\}$ be a function of the lattice sites, and define a lattice Laplacian Δ by $(\Delta f)_u = \sum_v \lambda_{uv}(f_v - f_u)$. We let $\varphi = \{\varphi_u\}$ be the unique solution [16] of the Poisson equation $-(\Delta\varphi)_u = q(\delta_{x,u} - \delta_{y,u})$ with a zero-point condition $\varphi_y = 0$. The "charge" $q > 0$ will be determined later. By using the periodicity of λ_{uv} and explicitly writing down the solution in terms of the Fourier series, one finds that φ has the following two properties [5]. P1) There exists a finite constant δ, and $|\varphi_u - \varphi_v| \le q\delta$ holds for any u, v with $|u - v| < R$. P2) In the $L \to \infty$ limit, one has $\varphi_x \ge q\gamma|x - y|$ in one dimension and $\varphi_x \ge q\alpha \ln|x - y|$ in two dimensions for sufficiently large $|x - y|$ with finite constants γ, α.

Noting that the above property P1) implies $\cosh(\varphi_u - \varphi_v) - 1 \le g(q)(\varphi_u - \varphi_v)^2$ for $|u - v| < R$ with $g(q) = \{\cosh(q\delta) - 1\}/(q\delta)^2$, we have

$$\|\exp[-\beta U]\|_\infty \le \exp\left[\beta \sum_{u,v} |t_{uv}[\cosh(\varphi_u - \varphi_v) - 1]|\right]$$

$$
\begin{aligned}
&\leq \exp\left[\beta g(q) \sum_{u,v} \lambda_{u,v} (\varphi_u - \varphi_v)^2\right] \\
&= \exp\left[-2\beta g(q) \sum_{u} \varphi_u (\Delta\varphi)_u\right] \\
&= \exp\left[2\beta g(q) q \varphi_x\right], \qquad (17)
\end{aligned}
$$

where we have used $\|c^\dagger_{u,\sigma} c_{v,\sigma} + c^\dagger_{v,\sigma} c_{u,\sigma}\|_\infty = 1$ to get the first bound. By substituting the bounds (14) and (17) into (8), we get

$$
|\langle A \rangle_L| = \frac{\left|\mathrm{Tr}[A e^{-\beta H}]\right|}{\mathrm{Tr}[A e^{-\beta H}]} \leq \exp[-2\varphi_x + 2\beta g(q) q \varphi_x]. \qquad (18)
$$

To optimize this bound, we define

$$
f(\beta) = \max_{q \geq 0} [2q - 2\beta\delta^{-2}\{\cosh(q\delta) - 1\}], \qquad (19)
$$

which is manifestly decreasing in β, and has the asymptotic behavior stated in the theorem. By using the property P2) of φ and letting the "charge" q to be the maximizer in the above, we finally get

$$
\left|\left\langle c^\dagger_{x,\uparrow} c^\dagger_{x,\downarrow} c_{y,\uparrow} c_{y,\downarrow} + \mathrm{H.c.} \right\rangle\right| \leq \begin{cases} \exp[-f(\beta)\gamma |x-y|] & \text{if } d = 1; \\ \exp[-f(\beta)\alpha \ln |x-y|] = |x-y|^{-\alpha f(\beta)} & \text{if } d = 2, \end{cases} \qquad (20)
$$

for sufficiently large $|x - y|$. Thus the bound (4) has been proved.

The bound (5) is proved in exactly the same manner. To prove the bound (6), we set $A = S^+_x S^-_y$, and perform a spin-dependent unitary transformation represented by $G(\theta) = \prod_{u,\sigma} \exp[-i\sigma\theta_u n_{u,\sigma}]$. The rest of the proof proceeds in exactly the same way as the above.

We wish to thank Elliott Lieb for letting us know the reference [4].

Note added (September 1997): In [17], extensions of our results to models with long range hopping was discussed.

References

[1] E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).

T. Koma, Prog. Theor. Phys. **83**, 655 (1990).

[2] E. H. Lieb, Phys. Rev. Lett. **62**, 1201 (1989).

Related general bounds have been proved in K. Kubo and T. Kishi, Phys. Rev. **B41**, 4866 (1990).

[3] Y. Nagaoka, Phys. Rev. 147, 392 (1966).

D. J. Thouless, Proc. Phys. Soc. London **86**, 893 (1965).

H. Tasaki, Phys. Rev. **B40**, 9192 (1989).

[4] D. K. Ghosh, Phys. Rev. Lett. 27, 1584 (1971).

[5] O. A. McBryan and T. Spencer, Commun. Math. Phys. **53**, 299 (1977).

[6] C. N. Yang, Phys. Rev. Lett. **63**, 2144 (1989).

[7] Note that an arbitrary one or two dimensional lattice can be mapped onto $\mathbf{Z}$ or $\mathbf{Z}^2$ with suitably modified hopping matrix elements.

[8] By using the technique developed in [11], it is possible to treat long ranged t_{xy}. In this case, however, the upper bounds decay much slower than power laws.

[9] In the translation invariant model with uniform nearest neighbor hopping t, we have $\gamma = \delta = 1/t$ in one dimension, and $\alpha = (2\pi t)^{-1}$ and $\delta = 4/t$ in two dimensions.

[10] It is easy to prove a bound similar to (4) for more complicated pairing function $\left\langle (P_x)^\dagger P_y \right\rangle$ with $P_x = c_{x,\sigma_1} c_{x+\delta_2,\sigma_2} \cdots c_{x+\delta_n,\sigma_n}$ where $\delta_2, \ldots, \delta_n$ are fixed lattice vectors and $\sigma_1, \ldots, \sigma_n$ are fixed spin indices. This allows us to rule out the condensation of various types of electron pairings. In a t-J model with the Hamiltonian

$$H = -\sum_{x,y,\sigma} t_{x,y} c^\dagger_{x,\sigma} c_{y,\sigma} + \sum_{x,y} J_{xy} \mathbf{S}_x \cdot \mathbf{S}_y + V(\{n_{x,\sigma}\}) \tag{21}$$

with t_{xy} satisfying the same conditions as before, we can prove the bounds (4), (5) (where the on-site singlet pair in (4) should be replaced by a suitable off-site singlet pair) for completely arbitrary J_{xy}, and the bound (6) for short ranged and uniformly bounded J_{xy}.

[11] K. R. Ito, J. Stat. Phys. **29**, 747 (1982).

Although Ito's paper is mainly devoted to the extension of McBryan-Spencer method to models with long-ranged interactions, it contains basic idea for extending the method to quantum spin systems. By using Ito's idea, one can prove the bound (6) (and the corresponding bound in one dimension) for a large class of quantum spin systems with short range interaction which is invariant under the global rotation about the z-axis. Our method, of course, applies to quantum spin systems, and is slightly simpler than Ito's.

[12] For related rigorous results, see J. Fröhlich and C. Pfister, Commun. Math. Phys. **81**, 277 (1981).

[13] N. D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1966).

[14] We prove the inequality for a positive integer m by an argument similar to that of Golden [15]. Let $\alpha_n = O^{2^{m-n}}(O^*)^{2^{m-n}}$ and $\beta_n = (O^*)^{2^{m-n}}O^{2^{m-n}}$ which are hermitian. Note that we have $\mathrm{Tr}[(\alpha_n)^N] = \mathrm{Tr}[(\beta_n)^N] = \mathrm{Tr}[(\alpha_{n+1}\beta_{n+1})^N]$. The inequality to be proved is $\mathrm{Tr}[\alpha_0] \le \mathrm{Tr}[(\alpha_m)^{2^m}]$. By using i) and $\mathrm{Tr}[(AB)^{2^k}] \le \mathrm{Tr}[A^{2^k}B^{2^k}]$ with A, B hermitian [15], we find for $0 \le k \le m-1$ that

$$\begin{aligned} \mathrm{Tr}[(\alpha_k)^{2^k}] &= \mathrm{Tr}[(\alpha_{k+1}\beta_{k+1})^{2^k}] \\ &\le \mathrm{Tr}[(\alpha_{k+1})^{2^k}(\beta_{k+1})^{2^k}] \\ &\le \mathrm{Tr}[(\alpha_{k+1})^{2^{k+1}}], \end{aligned} \tag{22}$$

which proves the desired bound.

[15] S. Golden, Phys. Rev. **137**, B1127 (1965).

K. Symanzik, J. Math. Phys. **6**, 1155 (1965).

C. J. Thompson, J. Math. Phys. **6**, 1812 (1965).

For a modern proof, see Appendix B of E. H. Lieb and W. Thiring, in *Studies in Mathematical Physics*, E. H. Lieb et al. eds., p.269. (Princeton University Press, 1976).

[16] The Laplacian Δ is not invertible since it has a zero mode f_u = const. However the Perron-Frobenius theorem ensures that the null space is one dimensional, and hence the Poisson equation with vanishing total charge has a unique solution.

[17] N. Macris and J. Ruiz, J. Stat. Phys. **75**, 1179 (1994).